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Band Engineering and Magnetic Doping of Epitaxial Graphene on SiC (0001) BYOUNG DON KONG, THUSHARI JAYASEKERA, KI WOOK KIM, M. BUONGIORNO NARDELLI, North Carolina State University — Advances in the epitaxial growth of graphene films on SiC have the potential to open new classes of device applications that may revolutionize the semiconductor roadmap for future decades. However, this progress will require an in-depth understanding and utilization of the electronic processes that take place at the nanoscale, in particular the role of the interface buffer layer, where most of the electronic properties of the system can be controlled. In analogy with the formation of the Schottky barrier in metal-insulator interfaces (the energetic barrier the electrons have to overcome to go from the valence band of the metal to the conduction band of the insulator) here we demonstrate the ability to tune and control the band alignment and the magnetic doping at the heterojunction between graphene and SiC, a fundamental requirement for improving device efficiency and applicability. Using first principles calculations, we will show how the surface electrostatic distribution can be used to tune the valence band offset by introducing surface impurities such as B, Al, N, and P. Similarly, we will demonstrate how the introduction of magnetic impurities in the buffer layer can tune the spintronic behavior of the epitaxial graphene layer. This work was supported, in part, by the NERC/NIST SWAN-NRI and the DARPA/HRL CERA programs.

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